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Strain-dependence of the superconducting critical temperature Tc in Al and Nb simple crystals from first-principles M. SALVETTI, N. BONINI, M.I.T., M. CALANDRA, IMPMC/CNRS, D. PARKS, N. MARZARI, J. MINERVINI, M.I.T. — In the past 20 years, efforts have been devoted to predict the critical current density J_c of superconducting magnets based on the Nb_3Sn compound. The use of Nb_3Sn magnets for high-field applications has highlighted the dependence of J_c on strain. We present calculations of the T_c-dependence of Al and Nb crystals on pressure, uni-axial and shear strains using the DFT *PWscf* package from the Quantum-ESPRESSO distribution to evaluate the phonon linewidth and the *el-ph* coupling parameter using very dense $\boldsymbol{k}$-space samplings of the IBZ. The superconducting critical T_c is calculated by using the McMillan formula as a fit to the solution of the Migdal-Eliashberg equations. Favourable comparisons with available experimental data have been obtained and will be presented. The modelling of the T_c-dependence on strain in Nb_3Sn crystals is an ongoing effort. The potential for modelling the T_c-dependence on strain in Nb_3Sn is discussed. In this regard, recent advances in the implementation of the Wannier formalism give access to the sampling of the dense $\boldsymbol{k}$-point grids required to calculate fully-converged electron-phonon coupling quantities. This approach opens the possibility to extend the study of the T_c-dependence on strain to unit cells characterized by a higher number of atoms or electronic complexity.

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